

Optical Conductivity in the Copper Oxide Materials

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Abstract

The frequency- and temperature-dependent optical conductivity of the copper oxide materials in the underdoped and optimal doped regimes are studied within the t - J model. The conductivity spectrum shows the unusual behavior at low energies and anomalous midinfrared peak in the low temperatures. However, this midinfrared peak is severely depressed with increasing temperatures, and vanishes at higher temperatures.

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After ten years of intense experimental study of the copper oxide superconductors, a significant body of reliable and reproducible data has been accumulated by using many probes [1,2], which shows that the most remarkable expression of the nonconventional physics of copper oxide materials is found in the normal-state [1,2]. The normal-state properties exhibit a number of anomalous properties in the sense that they do not fit in the conventional Fermi-liquid theory, and some properties mainly depend on the extent of dopings [1,2]. Among the striking features of the anomalous properties stands out the extraordinary optical conductivity [3]. The frequency- and temperature-dependent optical conductivity is a powerful probe for systems of interacting electrons, and provides very detailed information of the excitations, which interact with carriers in the normal-state and might play an important role in the superconductivity [3]. The optical conductivity of the copper oxide materials in the underdoped and optimally doped regimes has been extensively studied [3–6], and the experimental results indicate that the optical conductivity spectrum shows unusual behavior at low energies and anomalous midinfrared band in the charge-transfer gap, which is inconsistent with the conventional electron-phonon scattering mechanism.

Since the undoped copper oxide materials are antiferromagnetic Mott insulators, and upon doping with holes in the copper oxide sheets, the antiferromagnetic long-range-order (AFLRO) disappears and superconductivity emerges as the ground state [2], many researchers believe that the essential physics is contained in the doped antiferromagnets [7,8], which may be effectively described by the two-dimensional (2D) t - J model acting on the space with no doubly occupied sites. In spite of its simple form the t - J model proved to be very difficult to analyze, analytically as well as numerically, because of the electron single occupancy on-site local constraint. The local nature of the constraint is of primary importance, and its violation may lead to some unphysical results [9]. Recently a fermion-spin theory based on the charge-spin separation has been proposed to incorporate this constraint [10]. The main advantage of this approach is that the electron on-site local constraints can be treated exactly in analytical calculations. Within the fermion-spin theory, we [11] have shown that AFLRO vanishes around doping $\delta = 5\%$ for an reasonable value of the parameter

$t/J = 5$. The mean-field theory in the underdoped and optimally doped regimes without AFLRO has been developed [12], which has been applied to study the photoemission, electron dispersion and electron density of states in the copper oxide materials, and the results are qualitatively consistent with experiments and numerical simulations. In this paper, we consider fluctuations around this mean-field solution to study the optical conductivity, and show that the result within the fermion-spin formalism exhibits a behavior similar to that seen in the experiments and numerical simulations.

We begin with the t - J model defined on a square lattice,

$$H = -t \sum_{\langle ij \rangle \sigma} C_{i\sigma}^\dagger C_{j\sigma} + h.c. - \mu \sum_{i\sigma} C_{i\sigma}^\dagger C_{i\sigma} + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where $C_{i\sigma}^\dagger$ ($C_{i\sigma}$) are the electron creation (annihilation) operators, $\mathbf{S}_i = C_i^\dagger \boldsymbol{\sigma} C_i / 2$ are spin operators with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ as Pauli matrices, μ is the chemical potential, and the summation $\langle ij \rangle$ is carried over nearest nonrepeated bonds. Equation (1) is subject to an important constraint that a given site can not be occupied by more than one electron $\sum_\sigma C_{i\sigma}^\dagger C_{i\sigma} \leq 1$. This local constraint is satisfied even in the mean-field approximation within the fermion-spin transformation [10,12],

$$C_{i\uparrow} = h_i^\dagger S_i^-, \quad C_{i\downarrow} = h_i^\dagger S_i^+, \quad (2)$$

where the spinless fermion operator h_i keeps track of the charge (holon), while the pseudospin operator S_i keeps track of the spin (spinon). In this case, the t - J model (1) can be rewritten in the fermion-spin representation as,

$$H = -t \sum_{\langle ij \rangle} h_i h_j^\dagger (S_i^+ S_j^- + S_i^- S_j^+) + h.c. - \mu \sum_i h_i^\dagger h_i + J \sum_{\langle ij \rangle} (h_i h_i^\dagger) (\mathbf{S}_i \cdot \mathbf{S}_j) (h_j h_j^\dagger), \quad (3)$$

with S_i^+ and S_i^- as pseudospin raising and lowering operators, respectively. It is obvious that there is an interaction between spinons and holons in the Hamiltonian (3). The spinon and holon may be separated at the mean-field level, but they are strongly coupled beyond MFA due to fluctuations.

The mean-field theory within the fermion-spin formalism in the underdoped and optimally doped regimes without AFLRO has been developed [12], and the mean-field spinon

Green's function $D^{(0)}(i-j, \tau - \tau') = -\langle T_\tau S_i^+(\tau) S_j^-(\tau') \rangle_0$ and mean-field holon Green's function $g^{(0)}(i-j, \tau - \tau') = -\langle T_\tau h_i(\tau) h_j^\dagger(\tau') \rangle_0$ have been evaluated [12] as,

$$D^{(0)}(\mathbf{k}, \omega) = \frac{\Delta[(2\epsilon\chi_z + \chi)\gamma_k - (\epsilon\chi + 2\chi_z)]}{2\omega(k)} \left(\frac{1}{\omega - \omega(k)} - \frac{1}{\omega + \omega(k)} \right), \quad (4)$$

$$g^{(0)}(\mathbf{k}, \omega) = \frac{1}{\omega - \xi_k}, \quad (5)$$

respectively, where $\gamma_{\mathbf{k}} = (1/Z) \sum_{\eta} e^{i\mathbf{k} \cdot \hat{\eta}} \hat{\eta} = \pm \hat{x}, \pm \hat{y}$, $\Delta = 2ZJ_{eff}$, $J_{eff} = J[(1 - \delta)^2 - \phi^2]$, $\epsilon = 1 + 2t\phi/J_{eff}$, Z is the number of the nearest neighbor sites, the mean-field spinon excitation spectrum

$$\begin{aligned} \omega^2(k) = \Delta^2 & \left(\alpha\epsilon(\chi_z\gamma_k - \frac{1}{Z}\chi)(\epsilon\gamma_k - 1) + [\alpha C_z + \frac{1}{4Z}(1 - \alpha)](1 - \epsilon\gamma_k) \right) \\ & + \Delta^2 \left(\frac{1}{2}\alpha\epsilon\chi\gamma_k(\gamma_k - \epsilon) + \frac{1}{2}\epsilon[\alpha C + \frac{1}{2Z}(1 - \alpha)](\epsilon - \gamma_k) \right), \end{aligned} \quad (6)$$

and the mean-field holon excitation spectrum $\xi_k = 2Z\chi t\gamma_k - \mu$, with the spinon correlation functions $\chi = \langle S_i^+ S_{i+\eta}^- \rangle = \langle S_i^- S_{i+\eta}^+ \rangle$, $\chi_z = \langle S_i^z S_{i+\eta}^z \rangle$, $C = (1/Z^2) \sum_{\eta, \eta'} \langle S_{i+\eta}^+ S_{i+\eta'}^- \rangle$, $C_z = (1/Z^2) \sum_{\eta, \eta'} \langle S_{i+\eta}^z S_{i+\eta'}^z \rangle$, and holon particle-hole order parameter $\phi = \langle h_i^\dagger h_{i+\eta} \rangle$. In order not to violate the sum rule of the correlation function $\langle S_i^+ S_i^- \rangle = 1/2$ in the case without AFLRO, the important decoupling parameter α has been introduced in the mean-field calculation [12], which can be regarded as the vertex correlations [13]. The order parameters χ , C , χ_z , C_z , ϕ and chemical potential μ have been determined [12] by solving the self-consistent equations.

For discussing the optical conductivity, we now need to consider the fluctuations around the above mean-field solution. In the fermion-spin framework, an electron is represented by the product of a holon and a spinon, then the external field can only be coupled to one of them. Ioffe and Larkin [14] have shown that the physical conductivity $\sigma(\omega)$ is given by,

$$\sigma^{-1}(\omega) = \sigma_h^{-1}(\omega) + \sigma_s^{-1}(\omega), \quad (7)$$

where $\sigma_h(\omega)$ and $\sigma_s(\omega)$ are the contributions to the conductivity from holons and spinons, respectively, and can be expressed as [15],

$$\sigma_h(\omega) = -\text{Im}\Pi_h(\omega)/\omega, \quad \sigma_s(\omega) = -\text{Im}\Pi_s(\omega)/\omega, \quad (8)$$

with $\Pi_h(\omega)$ and $\Pi_s(\omega)$ as holon and spinon current-current correlation functions, respectively, and defined as,

$$\Pi_s(\tau - \tau') = -\langle T_\tau j_s(\tau) j_s(\tau') \rangle, \quad \Pi_h(\tau - \tau') = -\langle T_\tau j_h(\tau) j_h(\tau') \rangle, \quad (9)$$

where the current densities of spinons and holons are expressed in the present theoretical framework as,

$$j_s = te\phi \sum_{i\eta} \hat{\eta} (S_i^+ S_{i+\eta}^- + S_i^- S_{i+\eta}^+), \quad (10)$$

$$j_h = 2te\chi \sum_{i\eta} \hat{\eta} h_{i+\eta}^+ h_i, \quad (11)$$

respectively. In a formal calculation [16] for the spinon current-current correlation function we find $\Pi_s = 0$. However, the strongly correlation between holons and spinons is still considered through the spinon's order parameters χ , χ_z , C and C_z entering the holon current-current correlation function, which means that the holon moves in the background of spinons, and the cloud of distorted spinon background is to follow holons. Therefore the dressing of the holon by spinon excitations is the key ingredient in the explanation of the optical conductivity of the copper oxide materials.

The holon current-current correlation function defined in Eq. (9) can be rewritten as,

$$\Pi_h(i\omega_n) = -(2te\chi Z)^2 \frac{1}{N} \sum_k \gamma_{sk}^2 \frac{1}{\beta} \sum_{i\omega'_m} g(k, i\omega'_m + i\omega_n) g(k, i\omega'_m), \quad (12)$$

where $i\omega_n$ is the Matsubara frequency, $\gamma_{sk} = (1/2)(\sin k_x + \sin k_y)$, and $g(k, i\omega_n)$ is the full holon Green's function. In this paper, we consider the second-order correction for the holon. The second-order holon self-energy diagram from the spinon pair bubble has been discussed in Ref. [16], and the result was obtained as,

$$\begin{aligned} \Sigma_h^{(2)}(k, i\omega_n) = & (Zt)^2 \frac{1}{N^2} \sum_{pp'} (\gamma_{p'-k} + \gamma_{p'+p+k})^2 B_{p'} B_{p+p'} \times \\ & \left(2 \frac{n_F(\xi_{p+k}) [n_B(\omega_{p'}) - n_B(\omega_{p+p'})] - n_B(\omega_{p+p'}) n_B(-\omega_{p'})}{i\omega_n + \omega_{p+p'} - \omega_{p'} - \xi_{p+k}} \right. \\ & + \frac{n_F(\xi_{p+k}) [n_B(\omega_{p+p'}) - n_B(-\omega_{p'})] + n_B(\omega_{p'}) n_B(\omega_{p+p'})}{i\omega_n + \omega_{p'} + \omega_{p+p'} - \xi_{p+k}} \\ & \left. - \frac{n_F(\xi_{p+k}) [n_B(\omega_{p+p'}) - n_B(-\omega_{p'})] - n_B(-\omega_{p'}) n_B(-\omega_{p+p'})}{i\omega_n - \omega_{p+p'} - \omega_{p'} - \xi_{p+k}} \right), \end{aligned} \quad (13)$$

where $B_k = ZJ_{eff}[(2\epsilon\chi_z + \chi)\gamma_k - (\epsilon\chi + 2\chi_z)]/\omega_k$, $n_F(\xi_k)$ and $n_B(\omega_k)$ are the Fermi and Bose distribution functions, respectively. Then the full holon Green's function is obtained,

$$g(k, i\omega_n) = \frac{1}{g^{(0)-1}(k, i\omega_n) - \Sigma_h^{(2)}(k, i\omega_n)} = \frac{1}{i\omega_n - \xi_k - \Sigma_h^{(2)}(k, i\omega_n)}. \quad (14)$$

The above full holon Green's function $g(k, i\omega_n)$ can also be expressed as frequency integrals in terms of the spectral representation,

$$g(k, i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_h(k, \omega)}{i\omega_n - \omega}, \quad (15)$$

with the holon spectral function $A_h(k, \omega) = -2\text{Im}g(k, \omega)$. Substituting Eq. (15) into Eq. (12), and evaluating the frequency summations, we obtain the optical conductivity from Eqs. (7) and (8) as,

$$\sigma(\omega) = \frac{1}{2}(2te\chi Z)^2 \frac{1}{N} \sum_k \gamma_{sk}^2 \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A_h(k, \omega' + \omega) A_h(k, \omega') \frac{n_F(\omega' + \omega) - n_F(\omega')}{\omega}. \quad (16)$$

Although the optical properties of the copper oxide materials are very complicated, some qualitative features, such as (1) a sharp peak at $\omega = 0$, (2) considerable weight appears inside the charge-transfer gap of the undoped materials, defining the midinfrared band, and (3) the conductivity decays as $\rightarrow 1/\omega$ at low energies, seem to be common to all copper oxide materials [3,17]. In the following, we study the frequency- and temperature-dependent optical conductivity of the copper oxide materials in the underdoped and optimally doped regimes. We have performed a numerical calculation for the optical conductivity (16) at finite temperatures, and the results with temperature $T = 0.2J$ at dopings $\delta = 0.06$ (solid line), $\delta = 0.10$ (dashed line), and $\delta = 0.15$ (dot line) for the parameter $t/J = 2.5$ are plotted in Fig. 1, where the charge e has been set as the unit. Our low temperature results show that there is a low-energy peak at $\omega < 0.5t$ separated by a gap or pseudogap $= 0.5t$ from the broad absorption band (midinfrared band) in the conductivity spectrum. Moreover, The midinfrared spectral weight is doping dependent, increasing with doping for $0.5t < \omega < 2t$ and is nearly independent of doping for $\omega > 2t$. In particular, the midinfrared spectral weight is biased towards the lower energy region with increased doping. This reflects the increase in

the mobile carrier density, and indicates that the spectral weight of the midinfrared sideband is taken from the Drude absorption. Therefore the spectral weight from both the low-energy peak and midinfrared sideband represents the actual free-carrier density. These results are in qualitative agreement with experiments [4–6] and numerical simulations [18,19].

For further understanding the property of the optical conductivity, we show $\sigma(\omega)$ at (a) doping $\delta = 0.06$ and (b) $\delta = 0.15$ for $t/J = 2.5$ with temperatures $T = 0.2J$ (solid line), $T = 0.4J$ (dashed line), $T = 0.6J$ (dot-dashed line), and $T = 1.0J$ (dot line) in Fig. 2. In comparison with the low temperature result in Fig. 1, we find that the conductivity is temperature-dependent for $\omega < 1.5t$ and almost temperature-independent for $\omega > 1.5t$. The peak at $\omega = 0$ broadens and decreases in height with increasing temperatures, and the component in the low-energy region also increases with increasing temperature. Therefore there is a tendency towards the Drude-like behavior, while the midinfrared spectral weight (centered near $\omega \approx 1t$) is severely suppressed with increasing temperatures, and vanishes at higher temperatures ($T > 0.5J$), which are also consistent with the numerical simulations [20] and experiments [4–6,21]. Although the midinfrared spectral weight vanishes at higher temperatures, the total spectral weight of the optical conductivity does not change since the midinfrared spectral weight has been incorporated into the low-energy spectral weight, and therefore the sum rule of the optical conductivity [22] is still satisfied. In the present fermion-spin theory based on the charge-spin separation, the basic low-energy excitations are holons and spinons, but our theoretical results show that the anomalous optical properties at finite temperature are mainly caused by the charged holons in the copper oxide sheets, which are strongly renormalized because of the strong interactions with fluctuations of the surrounding spinon excitations.

In summary, we have studied the frequency- and temperature-dependent optical conductivity of the copper oxide materials in the underdoped and optimally doped regimes within the t - J model, and the theoretical results of the optical conductivity at finite temperatures are qualitatively consistent with experiments [5,21] and numerical simulations [18,20]. Our optical spectra have been used to extract the dc conductivity and resistivity [16], and the

result shows that the resistivity indeed exhibits a very good linear behavior at low temperatures in the underdoped and optimally doped regimes.

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REFERENCES

Mailing address.

- [1] See, e. g., B. Batlogg, in *High Temperature Superconductivity*, Proc. Los Alamos Symp., 1989, edited by K. S. Bedell, D. Coffey, D. E. Meltzer, D. Pines, and J. R. Schrieffer (Addison-Wesley, Redwood City, California, 1990); B. Batlogg, H. Y. Hwang, H. Takagi, R. J. Cava, H. L. Kao, and J. Kwo, *Physica C* **235-240**, 130 (1994).
- [2] A. P. Kampf, *Phys. Rep.* **249**, 219 (1994), and references therein.
- [3] D. B. Tanner and T. Timusk, in *Physical Properties of High Temperature Superconductors* III, edited by D. M. Ginsberg (World Scientific, Singapore, 1992), p. 363.
- [4] T. Timusk, M. Reedyk, R. Hughes, D. A. Bonn, J. D. Garret, J. E. Greedan, C. V. Stager, D. B. Tanner, Feng Gao, S. L. Herr, K. Kamaras, G. A. Thomas, S. L. Cooper, J. Orenstein, L. F. Schneemeyer, and A. J. Millis, *Physica C* **162-164**, 841 (1989); S. Uchida, T. Ido, H. Takagi, T. Arima, Y. Tokura, and S. Taima, *Phys. Rev. B* **43**, 7942 (1991).
- [5] S. L. Cooper, D. Reznik, A. Kotz, M. A. Karlow, R. Liu, M. V. Klein, B. W. Veal, and P. Paulikas, *Phys. Rev. B* **47**, 8233 (1993); A. V. Puchkov, P. Fournier, T. Timusk, and N. N. Kolesnikov, *Phys. Rev. Lett.* **77**, 1853 (1996).
- [6] N. W. Preyer, R. J. Birgeneau, C. Y. Chen, D. R. Gabbe, H. P. Jenssen, M. A. Kastner, P. J. Picone, and T. Thio, *Phys. Rev. B* **39**, 11563 (1989).
- [7] P. W. Anderson, in *Frontiers and Borderlines in Many Particle Physics*, edited by R. A. Broglia and J. R. Schrieffer (North-Holland, Amsterdam, 1987), p. 1; *Science* **235**, 1196 (1987).
- [8] F. C. Zhang and T. M. Rice, *Phys. Rev. B* **37**, 3759 (1988).
- [9] L. Zhang, J. K. Jain, and V. J. Emery, *Phys. Rev. B* **47**, 3368 (1993); Shiping Feng, J.

- B. Wu, Z. B. Su, and L. Yu, Phys. Rev. B **47**, 15192 (1993).
- [10] Shiping Feng, Z. B. Su, and L. Yu, Phys. Rev. B **49**, 2368 (1994); Mod. Phys. Lett. B **7**, 1013 (1993).
- [11] Shiping Feng, Yun Song, and Zhongbing Huang, Mod. Phys. Lett. B **10**, 1301 (1996); Commun. Theor. Phys. **29**, 187 (1998).
- [12] Shiping Feng and Yun Song, Phys. Rev. B **55**, 642 (1997).
- [13] J. Kondo and K. Yamaji, Prog. Theor. Phys. **47**, 807 (1972); H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **60**, 2394 (1991).
- [14] L. B. Ioffe and A. I. Larkin, Phys. Rev. B **39**, 8988 (1989).
- [15] G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
- [16] Shiping Feng and Zhongbing Huang, in *Proceedings of the International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors*, edited by Y. S. He, P. H. Wu, L. F. Xu, and Z. X. Zhao [Physica C **282-287**, 1687 (1997)]; Phys. Lett. A **232**, 293 (1997).
- [17] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994); and references therein.
- [18] W. Stephan and P. Horsch, Phys. Rev. B **42**, 8736 (1990).
- [19] A. Moreo and E. Dagotto, Phys. Rev. B **42**, 4786 (1990).
- [20] J. Jaklič and P. Prelovšek, Phys. Rev. B **50**, 7129 (1994).
- [21] J. Orenstein, G. A. Thomas, A. Millis, S. L. Cooper, D. Rapkin, T. Timusk, L. Schneemeyer, and J. Waszczak, Phys. Rev. B **42**, 6342 (1990).
- [22] F. Stern, *Solid State Physics* (Academic, New York, 1963), Vol. 15.

FIGURES

FIG. 1. The optical conductivity at the doping $\delta = 0.06$ (solid line), $\delta = 0.10$ (dashed line), and $\delta = 0.15$ (dot line) for the parameter $t/J = 2.5$ with the temperature $T = 0.2J$.

FIG. 2. The optical conductivity at (a) the doping $\delta = 0.06$ and (b) $\delta = 0.15$ for the parameter $t/J = 2.5$ with temperatures $T = 0.2J$ (solid line), $T = 0.4J$ (dashed line), $T = 0.6J$ (dot-dashed line), $T = 1.0J$ (dot line).